THRESHOLD IONIZATION SPECTROSCOPY AND SPIN-ORBIT COUPLING OF CeC_3H_4 and CeC_3H_6 FORMED in Ce + PROPENE REACTION

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CeC_3H_4 and CeC_3H_6 are observed in the reaction of Ce with propene in molecular beams and characterized by mass-analyzed threshold ionization (MATI) spectroscopy and relativistic quantum calculations. The MATI spectrum of each species displays two band systems, each consisting of vibronic progressions from Ce-C stretching and ligand bending excitations in the ionic states. The adiabatic ionization energies of CeC_3H_4 and CeC_3H_6 are 41035 (5) and 41868 (5) cm^{-1}, respectively. The two band systems are separated by 125 $\mathrm{cm}^{-1}$for CeC_3H_4 and 60 $\mathrm{cm}^{-1}$for CeC_3H_6. By comparing the splittings from the spectra with the relativistic calculations at the level of multiconfiguration quasi-degenerate second-order perturbation theory, we assign the two band systems to transitions from two spin-orbit levels of the neutral molecules.